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Abstract

This paper is devoted to an intercomparison of ozone vertical profiles retrieved from the measurements of scattered solar radiation performed by the SCIAMACHY instrument in the limb viewing geometry. Three different inversion algorithms including the prototype of the operational Level 1 to 2 processor to be operated by the European Space Agency are considered. The intercomparison was performed for 5 selected orbits of SCIAMACHY showing a good overall agreement of the results in the middle stratosphere, whereas considerable discrepancies were identified in the lower stratosphere and upper troposphere altitude region. Additionally, comparisons with ground-based lidar measurements are shown for selected profiles demonstrating an overall correctness of the retrievals.

1 Introduction

The Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) (Bovensmann et al., 1999) launched on board the European Environment Satellite (ENVISAT-1) in March 2002 is one of the new-generation space-borne instruments capable of performing spectrally resolved limb measurements of the solar radiation scattered in the Earth's atmosphere. This novel remote sensing technique allows daily near-global measurements of the atmospheric composition from space with high vertical resolution (2–3 km) (McPeters et al., 2000; von Savigny et al., 2003, 2005b; Rozanov et al., 2005a).

Retrievals of limb measurements performed by space-borne instruments launched previously as well as first retrievals of SCIAMACHY measurements demonstrate a huge information content of scattered solar light observations performed in the limb viewing geometry. However, due to the complexity of the scattering processes which the solar light detected by limb-viewing space-borne instruments undergoes, the retrieval of atmospheric trace gases from limb measurements requires sophisticated forward modeling and inversion approaches. The SCIAMACHY instrument achieves a full global coverage in 6 days which results in a large amount of measured data requiring the operational retrieval algorithms to be numerically efficient.

In this paper three different algorithms aimed to retrieve the vertical distribution of ozone from SCIAMACHY limb measurements are considered. The first one based on the global fit method was developed at the German Aerospace Center (DLR) Oberpfaffenhofen on behalf of the European Space Agency to be used as a part of the operational Level 1 to 2 data processing chain. In the current study version 3.0 of the DLR retrieval processor was employed. The validation results of the precursor versions 2.4 and 2.5 of this retrieval processor were presented by Brinksma et al. (2006). The second algorithm based on the so-called triplet method was developed at the Institute of Environmental Physics of the University of Bremen to perform the routine retrieval of the ozone vertical profiles (von Savigny et al., 2005b). This method will be further referenced to as the Stratozone algorithm. Throughout this study version 1.62 of the Stratozone retrieval algorithm was employed. An extended database of vertical distributions of ozone retrieved for all available limb measurements performed since September 2002 until now using the Stratozone algorithm is available through the web site of the Institute of Environmental Physics[1]. The validation results of the precursor versions 1.6 and 1.61 of this retrieval processor were presented by Segers et al. (2005) and Brinksma et al. (2006), respectively. The third algorithm also based on the global fit method is a part of the SCIATRAN 2.1 software package (Rozanov, 2004-2006; Rozanov et al., 2005a,b) comprising the radiative transfer model and the retrieval module which was developed at the Institute of Environmental Physics of the University of Bremen as well. A detailed description of the retrieval processors will be presented in the next section.

[1] http://www.iup.physik.uni-bremen.de/scia-arc/

2 Retrieval processors

The retrieval problem in atmospheric remote sensing is to estimate vertical profiles of atmospheric parameters from spectroscopic measurements. From a computational point of view the basic problem is the inversion of the radiative transfer equation. The discretization of the radiative transfer equation leads to the data model:

$$\boldsymbol{y} = F(\boldsymbol{x}) \tag{1}$$

where the mapping F represents the forward model, $\boldsymbol{y}$ is the exact data vector and $\boldsymbol{x}$ is the state vector containing the atmospheric parameters (e.g., temperature or molecular density profiles) to be retrieved. Measurements are made to a finite accuracy and in practice only the noisy data vector

$$\boldsymbol{y}^{\delta} = \boldsymbol{y} + \delta, \tag{2}$$

is available. For simplicity, we assume that the measurement error δ is stochastic with zero mean and identity covariance matrix $\mathbf{S}_{\delta}=\mathbf{I}$. In general, if the measurement error is described by a symmetric and positive definite covariance matrix $\mathbf{S}_{\delta}$, we can obtain a "normalized" data model with identity covariance matrix by the prewhitening technique (Rodgers, 2000). The inverse ill-posed problem is solved in the least squares sense by means of Tikhonov regularization with a stochastic constraint. This stochastic version of Tikhonov regularization is equivalent to the optimal estimation method (Rodgers, 2000). Essentially, an approximate solution is computed by minimizing the regularized function

$$\mathcal{F}(\boldsymbol{x}) = \left\|F(\boldsymbol{x}) - \boldsymbol{y}^{\delta}\right\|^2 + (\boldsymbol{x} - \boldsymbol{x}_{\mathrm{a}})^T \mathbf{S}_{\mathrm{a}}^{-1} (\boldsymbol{x} - \boldsymbol{x}_{\mathrm{a}}), \tag{3}$$

where $\mathbf{S}_{\mathrm{a}}$ is the a priori covariance matrix and $\boldsymbol{x}_{\mathrm{a}}$ is the a priori state vector, the best beforehand estimator of the true solution. Assuming that the a priori covariance matrix is of the form $\mathbf{S}_{\mathrm{a}}=\sigma_{\mathrm{a}}^2\hat{\boldsymbol{S}}_{\mathrm{a}}$, where σ_{a} is the a priori standard deviation of the profile, we introduce the stochastic regularization matrix $\mathbf{L}$ (of rank n) by the Choleski factorization $\hat{\mathbf{S}}_a^{-1} = \mathbf{L}^T \mathbf{L}$, and rewrite the regularized function (3) as

$$\mathcal{F}(\boldsymbol{x}) = \left\|\boldsymbol{F}(\boldsymbol{x}) - \boldsymbol{y}^\delta\right\|^2 + \lambda_a^2 \left\|\mathbf{L}(\boldsymbol{x} - \boldsymbol{x}_a)\right\|^2 , \tag{4}$$

where $\lambda_a = 1/\sigma_a$ is the stochastic regularization parameter.

The processors applied for ozone retrieval use different data and radiative transfer models and employ different techniques for solving the minimization problem as given by Eq. (3) or Eq. (4).

1. The Stratozone SCIAMACHY limb processor exploits the differential absorption structure between the center and the wings of the Chappuis absorption band of ozone, centered at 600 nm (von Savigny et al., 2005b). The retrieval algorithm is based on the so-called triplet method developed by Flittner et al. (2000) that was originally used to retrieve stratospheric ozone profiles from limb scattered radiances measured by the SOLSE/LORE (Shuttle Ozone Limb Sounding Experiment/ Limb Ozone Retrieval Experiment) instrumentation (McPeters et al., 2000). A similar technique is also used to retrieve stratospheric ozone profiles from limb scatter measurements performed by the OSIRIS (Optical Spectrograph and InfraRed Imager System) instrument on board the Swedish satellite Odin (von Savigny et al., 2003). The limb radiance profiles $I(\lambda, s)$ averaged over 2 nm spectral intervals centered around λ_1=525 nm, λ_2=600, and λ_3=675 nm are normalized with respect to the limb radiance at a tangent height $s_{\mathtt{ref}}$:

$$I_n(\lambda, s) = \frac{I(\lambda, s)}{I(\lambda, s_{\mathtt{ref}})}, \; s \neq s_{\mathtt{ref}} . \tag{5}$$

The normalized limb radiance profiles are then combined to the so-called Chappuis vector defined by

$$F_C(s) = \frac{I_n(\lambda_2, s)}{\sqrt{I_n(\lambda_1, s)\, I_n(\lambda_3, s)}} \tag{6}$$

and the data model is formulated as follows:

$$\boldsymbol{y}^{\delta} = \boldsymbol{F}_{\mathtt{C}}^{\mathtt{meas}}, \tag{7}$$

$$\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{F}_{\mathtt{C}}^{\mathtt{sim}}, \tag{8}$$

where the synthetic Chappuis vector $\boldsymbol{F}_{\mathtt{C}}^{\mathtt{sim}}$ as well as the analytical weighting functions are calculated using the SCIARAYS radiative transfer model taking into account the refractive ray tracing and surface reflection (Kaiser and Burrows, 2003). Similar to the conventional optimal estimation method the minimization problem as given by Eq. (3) is solved iteratively using the Gauss–Newton method. Throughout this study version 1.62 of the Stratozone retrieval processor was employed.

2. Alternatively to the Stratozone algorithm routinely running at the University of Bremen, the SCIATRAN 2.1 retrieval package (Rozanov, 2004-2006) which employs the global fit approach was applied to retrieve the vertical distributions of ozone. The data model is expressed in terms of normalized limb radiances and relies on the DOAS (Differential Optical Absorption Spectroscopy) technique (Platt, 1994), i.e.,

$$\boldsymbol{y}^{\delta} = \ln\left(I_{\mathtt{n}}^{\mathtt{meas}}\right) - P_{k}^{\mathtt{meas}}, \tag{9}$$

$$\boldsymbol{F}(\boldsymbol{x}) = \ln\left(I_{\mathtt{n}}^{\mathtt{sim}}\right) - P_{k}^{\mathtt{sim}}, \tag{10}$$

where P_k is a polynomial of order k in λ, whose coefficients are obtained by fitting the function $\ln\left(I_{\mathtt{n}}\right)$ in the wavelength domain. Similar to the Stratozone method the normalization is done with respect to the limb spectrum measured at an upper tangent height and aimed to eliminate the solar Fraunhofer structure as well as the influence of the instrument response function, i.e., the need for an absolute instrument calibration. By subtracting lower-order polynomials from radiance spectra we remove those spectral features that are smoothly varying functions of wavelength, particularly those due to Rayleigh and Mie scattering. The differential absorption type model is very sensitive to weak absorptions and has a moderate degree of nonlinearity (the number of iterations required to achieve convergence does not exceed 4). The minimization problem is solved iteratively by using the truncated Levenberg–Marquardt method. The retrieval

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method is described in details in (Rozanov et al., 2005a) in application to the vertical profile retrieval of NO_2 and BrO. Essentially, at each iteration step, the a priori state vector is replaced by the state vector obtained at the previous iteration and the computed solution is projected onto the effective state space accessible with the measurement. This projection method aimed at an additional noise filtering was previously referred to as the Information Operator approach (Hoogen et al., 1999; Rozanov, 2001). In the framework of the SCIATRAN retrieval package, the radiative transfer model based on the combined differential-integral approach is employed to perform the forward simulations as well as to calculate appropriate weighting functions (Rozanov et al., 2001, 2005b).

3. The processor developed at the German Aerospace Center (DLR) Oberpfaffenhofen also uses the DOAS-type data model (9)–(10) and solves the minimization problem by using the iteratively Gauss-Newton method with a variable sequence of regularization parameters λ (Doicu et al., 2002). The strategy for choosing the regularization parameter relies on the L-curve criterion for each linear subproblem and allows enough regularization to be applied at the beginning of iterations and then to be gradually decreased. In fact, the initial value of the regularization parameters is computed by using the L-curve criterion and the decreasing sequence of regularization parameters is constructed by analyzing the reduction of the residual at the previous iteration. The radiative transfer model used by the DLR processor is a single-scattering model, while the multiple scattering effect is taken into account by using look-up table corrections (Flittner et al., 2000). Throughout this study version 3.0 of the DLR retrieval processor was employed.

3 General settings

The forward models incorporated in the considered retrieval processors were initialized using the climatological data base provided by C.A. McLinden (Personal communication), a constant surface albedo of 0.3, temperature dependent absorption cross sections of O_3 and NO_2 measured by the SCIAMACHY PFM Satellite Spectrometer (Bogumil et al., 1999) as well as the O_4 cross section from (Greenblatt et al., 1990). Furthermore, a pure Rayleigh atmosphere was assumed.

As discussed in Sect. 2 the Stratozone algorithm exploits the differential spectral signal in the entire Chappuis absorption band using the limb radiances averaged over 2 nm spectral intervals centered around 525, 600, and 675 nm. The limb radiances are normalized with respect to the limb measurement performed at about 49 km tangent height during the same limb sequence. Only limb measurements performed at tangent heights between 9 and 49 km are considered in the retrieval.

Both multispectral methods, i.e., SCIATRAN retrieval package of the University of Bremen and the retrieval processor of DLR, exploit the spectral information in 520 to 580 nm wavelength interval. The differential spectra are obtained subtracting the cubic polynomial from both measured and simulated data. Unlike the Stratozone method, the limb measurement performed at about 43 km tangent height during the same limb sequence is used as the reference spectrum and the set of limb measurements considered by the retrieval algorithm is restricted to the tangent height range between 14 and 40 km. To improve the retrieval quality the vertical columns of NO_2 and O_4 were estimated in combination with ozone retrievals using the same spectral information.

The diagonal elements of the a priori covariance matrices were selected in accordance with 100% a priori uncertainty for ozone and 20% a priori uncertainty for other atmospheric species if considered. The off-diagonal elements were obtained assuming a correlation length of 3.3 km. The measurement error covariance matrix was assumed to be diagonal with diagonal elements corresponding to a wavelength independent signal to noise ratio of 1000 for multispectral methods and 100 for the triplet method.

4 Sensitivity of limb measurements

Before the results of different retrieval processors will be discussed it is worth analyzing the overall sensitivity of ozone limb retrievals. This will allow us to select the altitude

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region where the influence of the retrieval parameters is not to high and, thus, the results of all three retrieval processors can be required to agree. The common way to analyze the sensitivity of the retrieval methods, which employ the optimal estimation technique or the Tikhonov regularization with an a priori parameter choice, is to look at the averaging kernels. In this case, the averaging kernels in the relevant altitude region are distinctly peaked at corresponding altitudes and the peak values can be used as a measure of the information content of the measurement at the corresponding altitude. Furthermore, the width of the averaging kernels provide an estimation of the vertical resolution of the measurements. However, the averaging kernel is a quantity which make sense only for the ordinary optimal estimation technique as introduced by (Rodgers, 2000) as well as for the Tikhonov regularization with a constant regularization parameter, i.e., for a priori parameter choice methods, whereas, for example, in the iteratively regularized Gauss-Newton method as employed in the DLR retrieval processor, the decreasing sequence of regularization parameters yields an identity averaging kernel. As pointed out by Doicu et al. (2007) in the information operator approach as employed by the SCIATRAN retrieval processor the regular representation for the averaging kernels as introduced by Rodgers (2000) is no more valid and should be rewritten using the truncated gain matrix. Furthermore, as the Levenberg-Marquardt method is used, the averaging kernels characterize each particular iterative step only and are not representative for the whole retrieval process any more. Thus, only the Stratozone retrieval processor can be characterized by the averaging kernels in the common way. This is the reason why the investigation of the sensitivity of ozone limb retrievals will be done below on the basis of averaging kernels resulting from the Stratozone retrieval processor only. Nevertheless, the results of this investigation are expected to be representative for all three retrieval processors due to the fact that they use the same kind of information, i.e., multispectral measurements of the scattered solar radiation in the Chappuis absorption band in limb viewing geometry at nearly the same set of tangent heights, and the employed retrieval approaches are basically similar.

Since the regularization term commonly incorporates an information on the a priori profile, the sensitivity of the retrieval and, thus, the averaging kernels are also dependent on the a priori information. Therefore, the investigation below will be done for two different ozone profiles specific to the tropical and to the high latitude regions. Example profiles for 20 September 2004, typical for the fall in these latitude regions are shown in the left panel of Fig. 1. As clearly seen the high latitudinal profile exhibit much lower maximum altitude and much higher ozone number densities below 20 km as compared to the tropical profile. The corresponding averaging kernels are shown in the middle and the left panels of Fig. 1. The colored numbers on the right-hand side of the panels denote the altitudes which the averaging kernels were calculated for and the bold black bars indicate the tangent heights of the corresponding limb measurements. Since the measurements are performed with a tangent height sampling of about 3.3 km and the retrieval grid of 1 km spacing is used, the averaging kernels are expected to have the maximum values of 0.3 to 0.4 in the high sensitivity region.

Looking at the averaging kernels specific for the tropical region, as shown in the middle panel of Fig. 1, one clearly see that the maximum sensitivity is reached between 23 and 33 km where the peak values of the the averaging kernels are between 0.3 and 0.4, whereas between 19 and 23 as well as between 33 and 40 km they decrease to 0.2–0.25 indicating a partial loss of the sensitivity. However, these peak values are still high enough to obtain good retrieval results, although an increased dependence on a priori information can be expected. Below 19 km and above 40 km the maximum values of the averaging kernels are below 0.1 indicating a low information content of the measurements and strong dependence of the results on the a priori information.

As shown in the left panel of Fig. 1, quite different results are obtained for a high latitudinal profile. Here the maximum sensitivity region moves to 16–27 km altitude region, whereas between 13 and 16 km as well as between 27 and 30 km the peak values of the averaging kernels are still about 0.25 indicating a fair information content of the measurements. Between 30 and 40 km, where the peak values are between 0.1 and 0.2, the measurements still have a certain sensitivity, however, an increased influence of the a priori information is expected. Above 40 km, the averaging kernels drop below 0.05 and, thus, the retrieved values at these altitudes are expected to be dominated by a priori information.

Thus, basing on the discussion above, the target altitude region for the entire comparison can be selected as ~18–35 km, i.e., in this altitude region most of the measurements are considered to have a high information content and the results of all three retrieval processors are expected to agree.

5 Comparison of the retrieval processors

The comparison was performed for 5 selected orbits incorporating 104 individual limb measurements. To investigate possible discrepancies between the results of considered retrieval processors in different latitude regions three successive orbits in September 2004 with orbit numbers 13379, 13380, and 13381 were selected. Two additional orbits in January and March 2004 with orbit numbers 9816 and 10740, respectively, were selected to detect possible temporal variations in the closeness of agreement between the retrieval processors.

Figure 2 shows ozone profiles retrieved by different algorithms averaged over all limb states included in the comparison. The mean O_3 profile resulted from the Stratozone processor routinely running at the University of Bremen is presented by the red solid line. The green solid line represents the results obtained from operational limb processor developed by DLR and the blue solid line depicts the mean profile obtained using the SCIATRAN retrieval package. The corresponding standard deviation for the results of each retrieval processor is shown by the dotted line of appropriate color. As seen from the plot the methods are in a good agreement between 19 and 40 km. Below 19 km the sensitivity of the measurements gets worse and the influence on the retrieval initialization parameters increases.

Despite an overall agreement, the vertical fineness of the averaged profiles is different which is caused by the usage of different retrieval grids in different methods. The altitude steps of the retrieval grids were selected as 1.0 km in both Stratozone and SCI-

ATRAN, and 3.3 km in the DLR processor. This difference, however, is not expected to affect the vertical resolution of the retrieved profiles which is mainly determined by the instrument field of view (about 2.5 km at the tangent point) and by the vertical sampling of the SCIAMACHY limb measurements (about 3.3 km tangent height step). However, if the retrieval grid has finer layering than the tangent height sampling of the limb measurements, the algorithm is forced to perform some kind of interpolation in order to obtain the number densities between the measurement points. Thus, depending on the regularization method, the intermediate values of the number density can be estimated by the retrieval algorithm based on the overall vertical behavior of the profile. However, this approach can under the circumstances introduce fake vertical structures into the profiles. Additionally, the Information Operator approach employed in the SCIATRAN retrieval make these profiles vertically smoother compared to the results obtained by other methods introducing, however, larger smoothing error, see (Doicu et al., 2007) for details.

Figure 3 shows orbitally averaged ozone profiles retrieved by different algorithms in January, March, and September 2004. Each month is represented by one orbit and the averaging is performed over all limb measurements in the appropriate orbit. In all three seasons the profiles are in good agreement between 19 and 40 km. Below 19 km the agreement becomes worse similar to the comparison in Fig. 2. Generally, the Stratozone and the DLR retrieval exhibit similar vertical behavior down to 19 km differing by up to 12% between 23 and 26 km. In January and March the SCIATRAN retrievals are vertically smoother compared to the Stratozone results which can be explained by the additional smoothing specific to the retrieval method. However, in September both retrievals agree nearly perfectly above 18 km.

Figure 4 shows zonally averaged ozone profiles obtained from three orbits in September 2004. The largest disagreement between the different retrievals is encountered in the tropical region (20° S–20° N). Although the altitudes of the ozone maximum resulted from the different methods are in agreement, the Stratozone retrieval gives much larger altitude spread of the maximum concentration than found by two other methods. Furthermore, ozone concentrations obtained from the DLR retrieval above 23 km are systematically lower compared to the results of Statozone and SCIATRAN which also differ by up to 10% from each other. These discrepancies can be caused by different modeling of the scattering processes taking place in the Earth's atmosphere which are more complicated in the tropical region due to the high elevation of the Sun. Unlike previously discussed retrievals, the ozone number densities resulting from the SCIATRAN retrieval are noticeable smaller than the Stratozone and DLR results already below 20 km. This could be a results of a decreasing sensitivity to the lower layers because of high ozone content at high altitudes and low number densities below 20 km. As a result both Stratozone and DLR results tend to a priori values and the number densities resulted from the SCIATRAN retrieval are strongly affected by the values at higher altitudes. In the midlatitude regions (20° S–65° S and 20° N–65° N) of both Southern and Northern Hemisphere all retrievals agree very well. Although due to a finer retrieval grid both the Stratozone and the SCIATRAN retrievals look smoother compared to the DLR results, they do not seem to contain any additional information on the altitudinal behavior of the retrieved profiles. In the high latitude region of the Northern Hemisphere the Stratozone and SCIATRAN retrievals are in a very good agreement between 18 and 31 km. Below 18 km the values resulted from SCIATRAN retrieval are slightly lower compared to other methods, whereas above 31 km the Stratozone values are larger than DLR and SCIATRAN results. The DLR retrievals are in a very good agreement with SCIATRAN down to 24 km. Below this altitude the DLR profile seem to be shifted downwards by 1 to 1.5 km. In all latitudinal regions the agreement becomes worse below 18 km. The high latitude region of the Southern Hemisphere was not considered due to a small number of limb measurements.

6 Comparison to lidar measurements

In this section selected non-averaged ozone profiles retrieved from SCIAMACHY limb observations using different retrieval processors are compared with collocated ground-based lidar measurements. The lidar ozone measurements considered here are obtained by the differential absorption lidar (DIAL) method, in which the atmosphere is sounded vertically by two laser beams at wavelengths with different ozone absorption cross-section (e.g., McDermid et al., 1990, 1991, 1995). Range resolved measurements are obtained with the use of pulsed lasers. The spectral range of the laser beams is chosen in the ultraviolet where the ozone absorption is most efficient. The ozone number density is computed from the differentiation of the lidar signals (Godin et al., 1989, 1999; Godin-Beekmann et al., 2003). Due to the rapid decrease of the signal-to-noise ratio as a function of altitude, the retrieved ozone profile is smoothed with a low-pass filter characterized by a varying cutoff frequency as a function of altitude. The lidar measurements are performed during the night and last typically several hours. Owing to dynamic processes in the Earth's atmosphere, this results in a spatial resolution of about 100 km, depending on the atmospheric conditions. The vertical resolution ranges from several hundred meters in the lower range to several kilometers above 40 km. The total accuracy ranges from about a few percents below 20 km to more than 10% above 45 km.

The results of all three SCIAMACHY retrieval processors were shifted vertically by a pointing correction value of about –1.2 km as predicted by the TRUE algorithm (von Savigny et al., 2005a). Exact pointing correction values for all considered collocations are given below. The negative sign of the pointing correction value means that the corresponding profile is shifted downwards.

The results of the comparison are shown in Fig. 5. Similar to the previous plots the SCIAMACHY retrievals are represented by colored lines. For clarity reasons only each third error bar is drawn for all retrievals. The corresponding lidar measurement is shown by the solid black line with a shaded area representing the measurement uncertainty.

The left panel shows a comparison of ozone profiles retrieved from the SCIAMACHY limb measurement with average ground point coordinates 17.7° N, 155° W performed on 15 January 2004 at 20:20 UT with an ozone profile measured by the JPL-MLO lidar on 16 January 2004 at 05:44 UT over the Mauna Loa Observatory (19.54° N, 155.58° W). All SCIAMACHY profiles were shifted by a pointing correction value of –1.3 km. Although the overall agreement is quite good none of the SCIAMACHY retrievals is in a perfect agreement with the lidar profile. Both Stratozone and SCIATRAN retrievals seem to be vertically shifted by about 1 km with respect to the lidar profile. The DLR retrieval is in a very good agreement with the lidar ozone profile down to 24 km resulting, however, in too low values below. Despite the apparent vertical shift, the Stratozone algorithm reproduces the overall shape of the ozone profile very well although it seems to miss the small second maximum at 20 km. The SCIATRAN retrieval properly detects position of both main and secondary maxima but the absolute values of ozone concentrations resulted from the SCIATRAN retrieval are differing by 15–20% from the lidar profile due to contaminating oscillations which are apparently caused by an under-regularization of the retrieved profile.

The middle panel shows a comparison of ozone profiles retrieved from the SCIAMACHY limb measurement with average ground point coordinates 43° N, 14° E performed on 20 March 2004 at 09:28 UT with an ozone profile measured by the CNRS-OHP lidar on 19 March 2004 at 21:03 UT over the Observatoire de Haute-Provence (OHP, 44° N, 5.7° E). All SCIAMACHY profiles were shifted by a pointing correction value of –1.2 km. As seen from the plot, all retrievals produce similar results matching the overall shape of the lidar ozone profile and fail to reproduce the sharp peak at 19 km. Down to 21 km, all retrievals agree within 10–15% with each other and with the lidar ozone profile. The lack of ozone maximum at 19 km in all SCIAMACHY retrievals can either result from a coarse vertical sampling of the SCIAMACHY instrument (3.3 km tangent height step) in conjunction with an overall decrease of the retrieval sensitivity in the lower atmosphere or be caused by probing slightly different air masses. The latter is also in accordance with a high variability of the ozone vertical distribution in the lower stratosphere over OHP in the second half of March 2004. For example, high ozone concentration at about 19 km measured by the CNRS-OHP lidar on 19 March 2004 is probably due to an ozone-rich polar vortex filament moving over OHP at this time. To illustrate this high temporal variability the ozone profile measured by the CNRS-OHP lidar on 18 March 2004, i.e., one day before, is also shown in middle panel of Fig. 5 (brown line).

The right panel shows a comparison of ozone profiles retrieved from the SCIAMACHY limb measurement with average ground point coordinates 34.5° N, 119° W performed on 20 September 2004 at 18:10 UT with an ozone profile measured by the JPL-TMF lidar on 21 September 2004 at 06:14 UT over the Table Mountain Facility (34.4° N, 117.7° W). All SCIAMACHY profiles were shifted by a pointing correction value of –1.1 km. Similar to the previous plots, the shape of the ozone profiles retrieved from SCIAMACHY measurements agrees well with the shape of the lidar profile, although all SCIAMACHY retrievals exhibit less vertical structure compared to the lidar measurement. Obviously, this is caused by a partial loss of the information due to a coarse vertical sampling of the SCIAMACHY instrument. Down to 23 km all SCIAMACHY retrievals agree within 10–15% with each other and with the lidar ozone profile. However, below 23 km the agreement becomes worse due to a secondary maximum in the ozone profile resulting from the Stratozone retrieval.

7 Conclusions

Three different retrieval algorithms developed to gain vertical distributions of ozone from SCIAMACHY limb measurements are discussed. Two of them are the scientific algorithms developed at the University of Bremen and the third one is the prototype of the operational retrieval processor developed at the German Aerospace Center (DLR) in Oberpfaffenhofen on behalf of the European Space Agency. The results of different retrievals were compared with each other as well with independent ground-based lidar measurements.

The intercomparison shows that all retrieval methods are generally in a good agreement. Both zonally and orbitally averaged ozone profiles obtained with different retrieval algorithms agree within 10–15% down to 20 km. Below 19 km the information content of the limb measurements decreases with the altitude causing an increased influence of the retrieval constraints which results in larger deviations between different retrievals.

The comparisons of single ozone profiles retrieved from SCIAMACHY measurements using different retrieval methods with collocated ground-based lidar measurements show that the general shape of the ozone profiles and the retrieved amount of ozone is in good agreement although due to coarser vertical resolution the fine vertical structure of the profiles can not be obtained from the satellite measurements. The quantitative agreement between SCIAMACHY and lidar profiles can be estimated as 10–20% down to 22 km getting worse in the lower layers.

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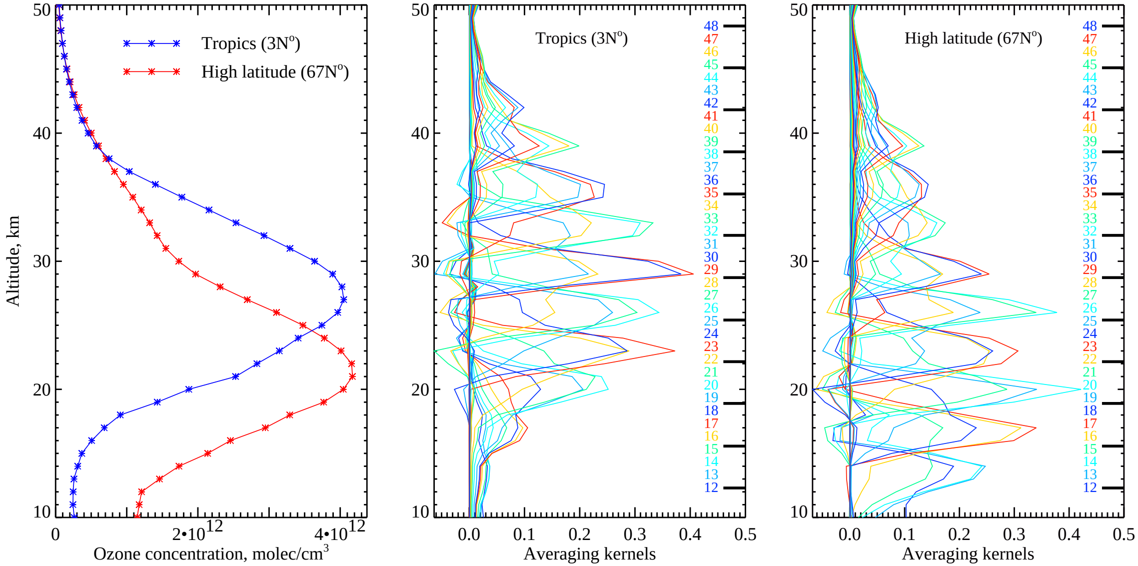

Fig. 1. Example ozone profiles for tropical and high latitude regions (left panel) as well as corresponding averaging kernels (middle panel for a tropical profile and right panel for a high latitudinal profile). The colored numbers on the right-hand side of the middle and right panels denote the altitudes which the averaging kernels were calculated for and the bold black bars indicate the tangent heights of the corresponding limb measurements.

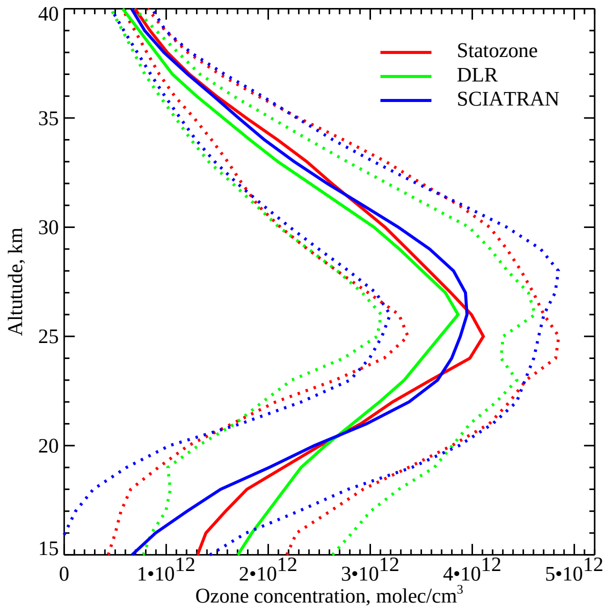

Fig. 2. Ozone profiles retrieved by different algorithms averaged over all limb states included in the comparison.

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7, 1969–1993, 2007

Comparison of the inversion algorithms

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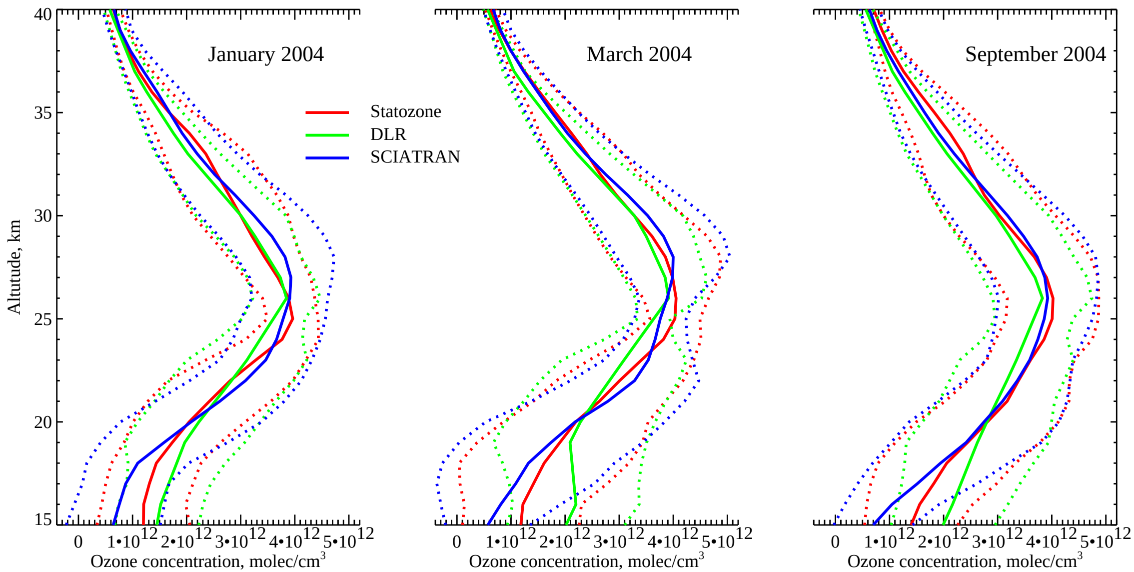

Fig. 3. Orbitally averaged ozone profiles retrieved by different algorithms in January, March, and September 2004.

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Comparison of the inversion algorithms

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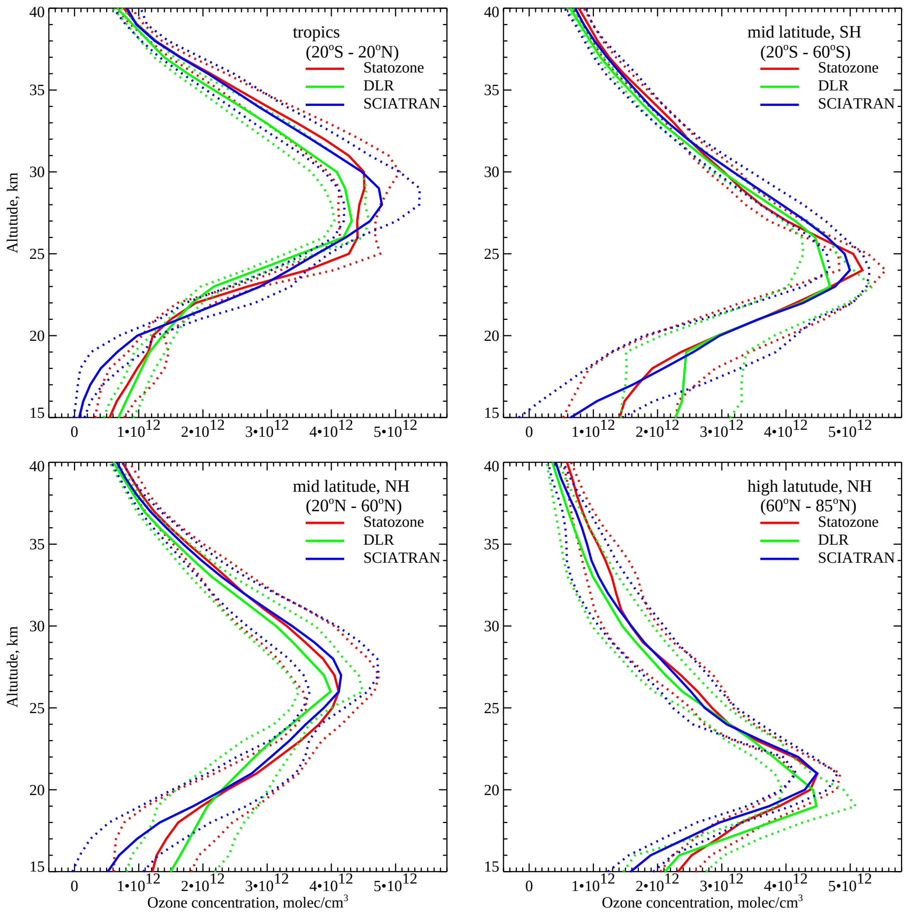

Fig. 4. Zonally averaged ozone profiles retrieved by different algorithms in September 2004.

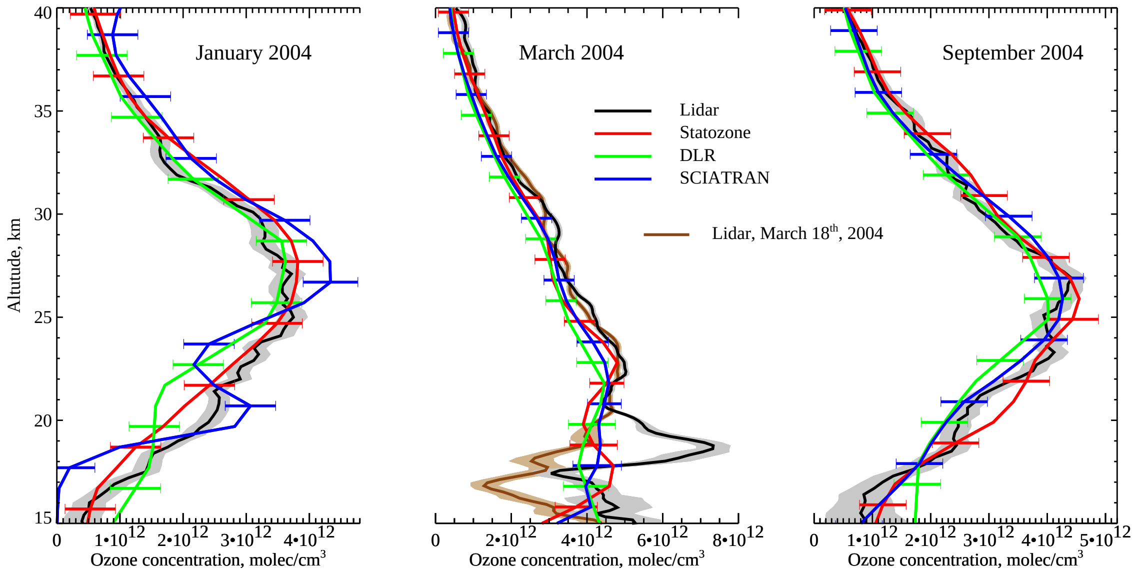

Fig. 5. Comparison to ground-based lidar measurements. Left panel: SCIAMACHY ozone profiles at average ground point coordinates 17.7° N, 155° W on 15 January 2004 at 20:20 UT compared to JPL-MLO lidar measurement at Mauna Loa Observatory (19.54° N, 155.58° W) on 16 January 2004 at 05:44 UT. Middle panel: SCIAMACHY ozone profiles at average ground point coordinates 43° N, 14° E on 20 March 2004 at 09:28 UT compared to CNRS-OHP lidar measurement at Observatoire de Haute-Provence (44° N, 5.7° E) on 19 March 2004 at 21:03 UT. To illustrate the high variability of the ozone vertical distribution, the CNRS-OHP lidar profile measured on 18 March 2004 is also shown (brown line). Right panel: SCIAMACHY ozone profiles at average ground point coordinates 34.5° N, 119° W on 20 September 2004 at 18:10 UT compared to JPL-TMF lidar measurement at Table Mountain Facility (34.4° N, 117.7° W) on 21 September 2004 at 06:14 UT.